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The light elements of the Earth's inner core

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We try to estimate the necessary amount of several light elements - C, S, P, O, Si - as major alloying components to match the observed seismic properties of the Earth's inner core. For this we compute the elastic constants tensors and determine the seismic properties of Fe$_3$X compounds, with X = C, S, P, O and Si, using first-principles calculations. Assuming linear relations and similar temperature corrections of velocities, we obtain as most reasonable carbon, silicon and/or oxygen.

Then we compute the electrical conductivity of iron and iron alloys at Earth's core conditions from electron-phonon coupling in the ABINIT implementation. We find an excellent agreement with experimental results for pure hcp iron below 1 mbars. We confidently use our results up to core pressure conditions. We show that the conductivity exhibits saturation at high pressures. We treat in detail the effect of Si on hcp iron and show a decrease of conductivity with Si concentration, an increase in anisotropy and a strong dependence with the substitution pattern.